

2'-Deoxyadenosine, 3'-O-TBDMS

Inchi: InChI=1S/C16H27N5O3Si/c1-16(2,3)25(4,5)24-10-6-12(23-11(10)7-22)21-9-20-13-14(17)
InchiKey: RZJNKNBLADNWHG-PQDIPPBSSA-N
Formula: C16H27N5O3Si
SMILES: CC(C)(C)[Si](C)(C)OC1CC(n2cnc3c(N)ncnc32)OC1CO
Mol. weight [g/mol]: 365.50

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.30 | | Crippen Method |
| logp | 2.079 | | Crippen Method |
| rinpol | 2731.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R246727&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/14-198-7/2-Deoxyadenosine-3-O-TBDMS.pdf>

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